HAMILTON CIRCUITS OF CONVEX TRIVALENT POLYHEDRA (UP TO 18 VERTICES)

BYJOSHUA LEDERBERG



Reprinted from the American Mathematical Monthly Vol. 74, No. 5, May, 1967

HAMILTON CIRCUITS OF CONVEX TRIVALENT POLYHEDRA (UP TO 18 VERTICES)

JOSHUA LEDERBERG, Stanford University School of Medicine

In a study of the graphs of chemical structures [1, 2], it became of interest to ascertain the Hamilton circuits (a closed circuit of edges through all the vertices) of trivalent graphs, and especially of the convex polyhedra. Tait [3] had conjectured that these polyhedra always had Hamilton circuits—for brevity we will now say had *circuits*. In [4], however, Tutte has demonstrated a counter-example with 46 vertices. Between about 12 or 14 vertices and 46, the territory has hardly been explored.

Grace [5] has recently presented a computer tabulation of the polyhedra through 18 vertices, affording a convenient opportunity to scan them for circuits, which were found in every instance. As Grace has noted, his criterion for isomorphism, "equisurroundedness" of the sets of faces is not strictly sufficient and his list may still be incomplete. As the isomorphism of *circuits* is fairly readily computed, this approach may be useful in further extensions of such studies.

The work needed to demonstrate a circuit is curtailed by the reducibility of any triangular face: A circuit through a triangle is equivalent to that through a node:



That is to say, to describe a circuit a triangular face can be shrunk down to a node. In effect, by induction, if all n-hedra have circuits, so will all (n+2)-hedra with triangular faces, and we need only examine those without. Table 1 shows that only 55 forms need to be studied.

Grace displayed the polyhedra as face-incidence lists. A computer program translated these into vertex-incidence lists. Each vertex being identified as a face-triple, those vertices are joined which share two faces. The vertex-incidence

TABLE 1. Count of Trivalent Convex Polyhedra

HAMILTON CIRCUITS OF CONVEX TRIVALENT POLYHEDRA

Vertices n	Faces f	Count Total [5]	Count No Triangles Present	Count No 3-connected Regions
4	4	1	. 0	0
6	5	1	0	0
8	6	2	1	1
10	7	5	1	1
12	8	14	2	2
14	9	50	5	4
16	10	233	12	10
18	11	1249	34	26
			_	_
		1555	55	44

list was then processed by a binary chained search of alternative paths; hence the search is always $\ll 2^n$, in contrast to the n! scope of a systematic permutation of the vertices. (A much more efficient algorithm has been discovered and is outlined as an appendix.)

Table 2 displays a circuit for each of the 55 polyhedra. The other polyhedra of order ≤18, and some of higher order can be developed from these by expanding nodes into triangles, a process that can be iterated.

The circuits lend themselves to a compact code from which the graph of a polyhedron is quickly constructed. Draw a polygon with vertices marked 1(1)n. Each successive character of the code denotes the span of a chord drawn from the next vacant vertex. Thus the prism would be 2, 3, 2 or BCB, and Hamilton's own example, the dodecahedron, is DJGDMJGDGD. There will be n/2 characters (to be sure the last one is redundant, being fixed by its predecessors). The letters A, B, $C \cdot \cdot \cdot$ stand for spans of 1, 2, $3 \cdot \cdot \cdot$ vertices. A and B do not appear in our list; A would connote a self-looped edge and B a triangular face.

Only one of the sometimes numerous circuits of each polyhedron is shown: it is merely the first one discovered by the computer search, but it has been placed in canonical form with respect to rotation and reflection of the polygon [2].

The complete list of the Hamilton circuits for each graph of Table 2 gives further insight into the composition of circuit-free graphs. Extracting one node from a polyhedron leaves a cut graph with three cut edges, e.g., a triangular region is the residue of a tetrahedron. In the first instance, in general such a residue will have the same facility for admitting a circuit as does an isolated node, depending on the set of circuits found in the polyhedron. Thus, except for CGDIGDFD (Grace's 16-55) all the polyhedra where $n \le 16$ have this property. Hence for finding circuits, any other 3-connected region can be replaced by a single node. By induction only the 44 forms counted in Table 1 need be considered for $n \le 18$.

CGDIGDFD, (Fig. 1a) which is the same as Tutte's graph N_2 [4], has three (symmetrically equivalent) edges that are obligatory in any Hamilton circuit. It is the simplest with such a property.

Tutte produced a 46-node circuit-free graph by replacing three nodes of a tetrahedron with 3 15-node residues so that 3 obligatory edges converged on one node in a self-contradictory way. Along the same lines a 38-node, circuit-free graph can be composed by replacing two nodes of *CFDEC*, the pentagonal prism, with two 15-node residues so as to confront two obligatory edges with two that, as pointed out by Tutte, are mutually exclusive. In an independent study, David Barnette has already discovered this graph [6].

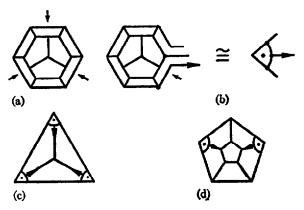


Fig. 1. Composition of non-Hamiltonian polyhedra. (a) 16CGDIGDFD which is Tutte's graph $N_2[4]$. The marked edges are obligatory in any circuit. (b) a 15-node residue with an obligatory edge as marked. (c) and (d) are two non-Hamiltonian polyhedra of 46 and 38 nodes respectively.

If we accept the enumeration of polyhedra for $n \le 16$, on which Grace concurs with Brückner [7], or merely that we know the 4-connected cases (as in table 2), a similar line of reasoning leads to an inferential argument for the conclusion that every 18-node polyhedron has a circuit. (We should say, more precisely, cyclically 4-connected as defined by Tutte [8]: "a cyclically k-connected graph cannot be broken up into two separate parts, each containing a polygon, by the removal of fewer than k edges.") Each of the graphs was searched by a computer program for subgraphs obtained by extracting any node-pair, and the circuit-forming properties of the subgraphs examined. None of the subgraphs was of a kind that would disqualify a pairwise combination of them from containing a circuit (cf. Tutte's arguments [8]). On the other hand, from Euler's formula, every 18-node polyhedron must (a) contain no 3-connected and at least one 4-connected subgraph which has 14 or fewer nodes, and would therefore fall within the scope of the search, or (b) is derived from a graph with at least one 3-connected region, a case already disposed of through n=16. The further

TABLE 2. Listing of Hamilton circuits

(Included are convex trivalent polyhedra with n≤18 vertices. Only polyhedra with no triangular face are listed. See text for code. Each character group stands for one polyhedron.)
* marks 3-connected forms; the remainder are 4-connected.

Vertex Count	Grace's Catalog [5] No.	Code	Vertex Count	Grace's Catalog [5] No.	Code
8	2	CECC	18	186	CNEMFCFCD
10	5	CFDEC		195	CNDMEGECE
12	6	CGEGEC		196	COLCGEIFC
	11	CHFCFD		198	CNKHLECHE
14	6	CJHECGE		233	CNDFCGDFD
	7	CJGDHFC		326	COEMIFCFC*
	8	CIGDHFD		328	CNDMDFDFC
	15	CHFIGEC		329	CNLDHECHD
	46	CKEIECC*		347	CNLDHFDHF
16	42	CMJFDIFC		348	CNLIFDJHC
	43	CLDKDECD		350	CODGEHFDE
	44	CLIFJCGD		353	CLJGDKIGD
	52	CLIFCIGC		354	CMJGLDIGD
	54	CLDECEEC		356	CODGDHFCE
	55	CGDIGDFD		362	CLJFDKIGC
	60	CLJGECHF		376	CNJGEKIFD
	61	CJHKDHFD		383	CNIFLJGEC
	62	CKIECIGC		392	COMCIFCHC*
8	70	CMKDGECF*		393	CNKHFDJHE
	88	CMDKFCEC*		401	COKHECJGC
	112	CIGKIGEC		418	CMKGEKIGC
				419	CMKHFDJHF
				426	CNLIGECIG
				427	CKIMKDHFD
	,			428	CMKGECJHC
				429	COCDGEHEC
				477	CNLDGECHC*
				493	COMELGECD*
				505	COCCEIECC
				508	CNGMKGECD*
				509	CODMHECFD*
				625	CODMCFCEC*
				626	CODMIECFC*
				887	CJHMKIGEC

application of this technique should make it possible to anticipate the smallest non-Hamiltonian polyhedron from the properties of the 4- and 5-connected polyhedra of the next lower order. Since these, by definition, all have circuits, it would be feasible to generate them on the computer by reasonably efficient combinatorial schemes to whatever order is required.

Appendix: Algorithm for finding Hamilton circuits of a cyclic graph.

This is illustrated for an undirected, trihedral graph but should be generalized without difficulty in an obvious way. The input is a description of the connectivity of the graph. The essence of the routine is to build a table of sets of edges so that just two edges incident on each node appear in any row of the table. The first node is chosen arbitrarily. Its three incident edges are marked current and open. The circuit-fragment table is started with three rows by listing the 3 pairwise choices among the current edges.

- 1. Select an open edge. The two adjacent edges become the trial edges.
- 2. How many trial edges match the current list: none, one, or two?
 - a. If none match, close the selected edge and replace it on the current open list by the two trial edges. Scan the circuit-fragment table. Each row in which the selected edge appears is replaced by two rows, one for each trial edge. Each remaining row is replaced by one row showing both trial edges. Go to 1.
 - b. If one matches, a circuit of the graph has been closed. Scan the circuit-fragment (c.f.) table contrasting the matched edge with the selected edge. Each c.f. where neither appears is deleted. If one of the two appears on a c.f., this is augmented by the trial edge. If both appear, the c.f. row stands as is unless a tracing of the c.f. shows it to be prematurely closed, whereupon it is deleted. Go to 1.
 - c. If both match two adjacent faces of the graph have been closed. The preceding subroutine is revised in an obvious way to close out both matched edges: those c.f. rows are retained which are compatible with the indicated edge allocations. Go to 1.

The process is terminated when the open edge list is vacated. If this leaves some nodes unused, no Hamilton circuit is possible. Otherwise, the final closure of circuit-fragments leaves a table of circuits. This must still be scanned to separate the Hamiltonian circuits from the set of pairwise disjoint circuits.

The efficiency of the algorithm depends on keeping the current c.f. table as small as possible. This is accomplished by a lookahead routine which scans prospective choices of current edges to seek the promptest closure of a face.

For an example, Tutte's 46 node non-Hamiltonian graph has been searched exhaustively. This required a c.f. table of 12,477 rows consuming 29 seconds of a program on IBM 7090. Searches yielding all the circuits of other large Hamiltonian graphs required a comparable effort.

This procedure may have some utility for studies on classification, isomorphisms, and symmetries of abstract graphs and other network problems for which the set of Hamilton circuits is often an advantageous approach. A complete description of the computer program is available from the author.

This work has been supported by a grant from NASA (NsG 81-60) for studies on automated experimental analysis. Computations were run on an IBM 7090 at the Stanford Computation Center with support from the National Science Foundation, under grant NSF-GP-948.

References

- 1. J. Lederberg, DENDRAL-64, A System for Computer Construction, Enumeration and Notation of organic Molecules as Tree Structures and Cyclic Graphs, Part I. (NASA Scientific and Technical Aerospace Report, STAR No. N65-13158, 1964, and CR 57029.)
 - 2. ——., Proc. Nat. Acad. Sci. U.S., 53 (1965) 134-139.
 - 3. P. G. Tait, Phil. Mag. (Series 5), 17 (1884) 30.
 - 4. W. T. Tutte, J. London Math. Soc., 21 (1946) 98.
- 5. D. W. Grace, Computer Search for Non-Isomorphic Convex Polyhedra, Stanford Computation Center Technical Report No. CS15 (1965).
 - 6. V. Klee, Personal communication.
 - 7. M. Brückner, Vielecke und Vielfläche, Teubner, Leipzig, 1900.
 - 8. W. T. Tutte, Acta Math. (Hung.), 11 (1960) 371.